EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** High resolution XRD measurements at low temperature of iodide-containing layered double hydroxides	**Experiment number:** **01-01-873**
Beamline: BM01B	**Date of experiment**: from: 13.05.11 to: 18.05.11	**Date of report**: 24.02.12
Shifts: 15	**Local contact(s)**: Hermann Emerich	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Laure Aimoz[1*], Dr. Erich Wieland[1], Dr. Christine Taviot Guého[2], Dr. Rainer Dähn[1], and Dr. Enzo Curti[1*]

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Report:

Results have been published in:

Laure Aimoz, Christine Taviot-Gueho, Sergey V. Churakov, Marina Chukalina, Rainer Daehn, Enzo Curti, Pierre Bordet, and Marika Vespa (2012). **Anion and Cation Order in Iodide-Bearing Zn/Mg-Al Layered Double Hydroxides *J. Phys. Chem. C*,** DOI: **10.1021/jp2119636**

Abstract:

Uptake of iodine in hydrotalcite-like minerals is a potential retardation mechanism for dose-relevant ^{129}I in the near-field of a deep repository for radioactive waste. The location of iodide in (Zn/Mg)Al layered double hydroxides (LDH) was investigated using a novel combination of advanced atomic-scale techniques. Wavelet transform analysis of Zn K-edge extended X-ray absorption fine structure (EXAFS) spectra and geometry optimization simulation based on ab initio calculations, allowed the distribution of Al^{3+} in the cationic layer to be determined. Using Rietveld refinement of synchrotron X-ray powder diffraction data (XRD) and EXAFS at the I K-edge enabled the average location of iodide in the interlayer to be established. Additional short- and medium-range structural information was also obtained from the pair distribution function analysis of the XRD data in support of the findings obtained with the long- and short-range techniques. By combining the results, a local order of Al^{3+} in Zn_2Al-I and Zn_3Al-I LDHs was shown generating hexagonal and orthorhombic supercells, respectively. Furthermore, an ordered distribution of trivalent and divalent cations in the hydroxide layer was demonstrated to have no influence on the distribution of iodide in the interlayer.